

# Spin-Gap Phase in the One-Dimensional $t$ - $J$ - $J'$ Model

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The spin-gap phase of the one-dimensional  $t$ - $J$ - $J'$  model is studied by the level-crossing of the singlet and the triplet excitation spectra. The phase boundary obtained between the Tomonaga-Luttinger and the spin-gap phases is remarkably consistent with the analytical results at the  $J, J' \rightarrow 0$  and the low-density limits discussed by Ogata *et al.* The spin-gap phase has a single domain in the phase diagram even if the spin gap opens at half-filling. The phase boundary coincides with the  $K_\rho = 1$  line where the Tomonaga-Luttinger liquid behaves as free electrons, in the low-density region. The relation between our method and the solution of the two-electron problem is also discussed.

**KEYWORDS:** Tomonaga-Luttinger liquid, spin gap, backward scattering, renormalization group, singlet-triplet level-crossing, twisted boundary conditions, factorized wave function, two-electron problem

The discovery of quasi one-dimensional (1D) cuprates has stimulated the study of 1D strongly correlated electron systems. The existence of a spin gap is an important factor to be considered in the investigation of superconductivity. The effect of frustration was considered to be a candidate causing a spin gap in the realistic parameter region. However, it was very difficult to determine the phase boundary between the Tomonaga-Luttinger (TL) and the spin-gap phases, due to the singular behavior of the spin gap near the critical point. Recently, the author with Nomura and Kitazawa have developed a new method to treat the spin gap, that is, the singlet-triplet level-crossing method with the twisted boundary conditions.<sup>1)</sup> In this letter, we will apply this method to the 1D  $t$ - $J$ - $J'$  model and show that the result is consistent with the exact results in the low-density and the  $J, J' \rightarrow 0$  limits, and we will clarify the spin-gap phase of this model.

The Hamiltonian of the 1D  $t$ - $J$ - $J'$  model is written in the subspace of no doubly occupied sites as

$$\mathcal{H} = -t \sum_{i\sigma} (c_{i\sigma}^\dagger c_{i+1\sigma} + \text{H.c.}) + \sum_{l=1,2} \sum_i J^{(l)} (\mathbf{S}_i \cdot \mathbf{S}_{i+l} - n_i n_{i+l}/4), \quad (1)$$

where  $J^{(1)} = J, J^{(2)} = J'$ . We also introduce a parameter  $\alpha$  for the strength of the frustration given by  $\alpha \equiv J'/J$ . At half-filling ( $n = 1$ ), this model becomes an  $S = 1/2$  frustrated spin chain. In this case, the ground state at  $\alpha = 1/2$  is the two-fold degenerate dimer state with a spin gap, and the ground state energy density is  $-3/4J$ .<sup>2,3,4)</sup> Okamoto and Nomura have argued, using the level crossing method, that the fluid-dimer transition occurs at  $\alpha_c = 0.2411$ .<sup>5)</sup> Upon doping of holes, the system may become metallic, and the spin gap is reduced<sup>6)</sup>

but persists for the finite doping. The phase diagram of this model for  $n \neq 1$  at  $\alpha = 1/2$ , using the exact diagonalization, was obtained by Ogata, Luchini and Rice.<sup>7)</sup> They also made an important achievement regarding the critical points for some limits.

We briefly review their method to obtain the critical points in the following two limits: in the limit of  $J, J' \rightarrow 0$ , the spin part of this model can be mapped onto the case of  $n = 1$ , using the factorized wave function,<sup>7,8)</sup>

$$J_{\text{eff}} = J \langle n_i n_{i+1} \rangle_{\text{SF}} + J' \langle n_i (1 - n_{i+1}) n_{i+2} \rangle_{\text{SF}}, \quad (2a)$$

$$J'_{\text{eff}} = J' \langle n_i n_{i+1} n_{i+2} \rangle_{\text{SF}}, \quad (2b)$$

where  $\langle \cdots \rangle_{\text{SF}}$  indicates the expectation value of the non-interacting spinless fermion. The effective ratio of the frustration  $\alpha_{\text{eff}}$  is then obtained as

$$\alpha_{\text{eff}}(n, \alpha) = \left[ \frac{(1 + 1/\alpha)n^2 - s_2^2 - s_1^2/\alpha}{n^3 - (2s_1^2 + s_2^2)n + 2s_1^2 s_2} - 1 \right]^{-1}, \quad (3)$$

where  $s_l \equiv \sin(l\pi n)/l\pi n$ . We can obtain the critical density  $n_c$  where the spin gap vanishes, by comparing eq.(3) with the value  $\alpha_c = 0.2411$  obtained by Okamoto and Nomura.<sup>5)</sup> For  $\alpha = 1/2$ ,  $n_c = 0.7433$ . On the other hand, for the low density limit, the critical value of  $J/t$  where the singlet pair forms a bound state, can be analytically obtained by solving the two-electron problem. The solution can be derived by adding a Hubbard interaction  $\mathcal{H}_U \equiv U \sum_i n_{i\uparrow} n_{i\downarrow}$  to the Hamiltonian, relaxing the constraint, and setting  $U = \infty$  at the end of the calculation.<sup>9)</sup> The obtained result is

$$\frac{J_c}{t} = \frac{1 + 2\alpha - \sqrt{1 + 4\alpha^2}}{\alpha}. \quad (4)$$

It is not trivial that this critical value is equivalent to the spin-gap phase boundary. We will discuss this point later.

The critical point in the remaining region can be determined in the following way.<sup>1)</sup> In this letter we argue within the scheme of the bosonization theory. The low

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energy behavior of 1D electron systems is described by the sine-Gordon model<sup>10,11)</sup>

$$\mathcal{H} = \mathcal{H}_\rho + \mathcal{H}_\sigma + \frac{2g_{1\perp}}{(2\pi a)^2} \int dx \cos(\sqrt{8}\phi_\sigma). \quad (5)$$

Here  $a$  is a short-distance cutoff,  $g_{1\perp}$  is the backward scattering amplitude and for  $\nu = \rho, \sigma$

$$\mathcal{H}_\nu = \frac{1}{2\pi} \int dx \left[ v_\nu K_\nu \left( \frac{\partial \theta_\nu}{\partial x} \right)^2 + \frac{v_\nu}{K_\nu} \left( \frac{\partial \phi_\nu}{\partial x} \right)^2 \right], \quad (6)$$

where  $v_\nu$  and  $K_\nu$  are the velocity and the Gaussian coupling, respectively, for the charge ( $\nu = \rho$ ) and the spin ( $\nu = \sigma$ ) sectors. In the TL phase ( $g_{1\perp} > 0$ ), the parameters  $K_\sigma$  and  $g_{1\perp}$  are renormalized as  $K_\sigma^* = 1$  and  $g_{1\perp}^* = 0$ , reflecting the SU(2) symmetry. The phase fields are defined as<sup>11,12)</sup>

$$\begin{aligned} \phi_\nu(x), \theta_\nu(x) = & \quad (7) \\ \mp \frac{i\pi}{L} \sum_{p \neq 0} \frac{1}{p} e^{-ia|p|/2 - ipx} [\nu_R(p) \pm \nu_L(p)] \mp n_\nu, m_\nu \frac{\sqrt{2}\pi x}{L}, \end{aligned}$$

where  $\nu_r$  is the charge ( $\nu = \rho$ ) or the spin ( $\nu = \sigma$ ) density operator, which satisfy the boundary conditions,

$$\phi_\nu(x+L) = \phi_\nu(x) - \sqrt{2}\pi n_\nu, \quad (8a)$$

$$\theta_\nu(x+L) = \theta_\nu(x) + \sqrt{2}\pi m_\nu. \quad (8b)$$

These phase fields have the relation  $[\phi_\nu(x), \partial_{x'} \theta_\nu(x')] = i\pi\delta(x-x')$ . The quantum numbers are defined by the total number operators (measured with respect to the ground state)  $N_{r\sigma}$  for right and left going particles ( $r = R, L$ ) of spin  $\sigma$ <sup>11,13)</sup>

$$n_\nu = [(N_{R\uparrow} + N_{L\uparrow}) \pm (N_{R\downarrow} + N_{L\downarrow})]/2, \quad (9a)$$

$$m_\nu = [(N_{R\uparrow} - N_{L\uparrow}) \pm (N_{R\downarrow} - N_{L\downarrow})]/2. \quad (9b)$$

Here the upper and lower sign refer to charge and spin degrees of freedoms, respectively. The selection rule among them for  $N = 4l + 2$  ( $l$ : integer) electrons in periodic boundary conditions is<sup>12,14)</sup>

$$(-1)^{m_\rho \pm m_\sigma} = (-1)^{n_\rho \pm n_\sigma}. \quad (10)$$

The finite-size corrections for the excitation energy and momentum of the system with length  $L$  are described by

$$E - E_0 = \frac{2\pi v_\rho}{L} x_\rho + \frac{2\pi v_\sigma}{L} x_\sigma, \quad (11)$$

$$P - P_0 = \frac{2\pi}{L} (s_\rho + s_\sigma) + 2m_\rho k_F, \quad (12)$$

where  $k_F = \pi n/2$  is the Fermi wave number,  $x_\nu \equiv (m_\nu^2 K_\nu + n_\nu^2 / K_\nu)/2$  and  $s_\nu \equiv m_\nu n_\nu$  are the scaling dimension and the conformal spin, respectively, for each sector. The corresponding operator is given by  $\exp[i\sqrt{2}(m_\nu \phi_\nu + n_\nu \theta_\nu)]$ . The boson representation of the fermion operator is

$$\psi_{r,\sigma} = \frac{1}{\sqrt{2\pi a}} e^{ir k_F x} e^{i/\sqrt{2}[\tau(\phi_\rho + \sigma \phi_\sigma) - \theta_\rho - \sigma \theta_\sigma]}, \quad (13)$$

where  $r = R, L$  and  $\sigma = \uparrow, \downarrow$  refer to  $+, -$  in that order.

Next we extract the singlet and the triplet excitation

spectra  $[m_\rho = n_\rho = 0, (m_\sigma, n_\sigma) = (1, 0), (0, \pm 1)]$ . The corresponding operators are  $\sqrt{2}\cos\sqrt{2}\phi_\sigma$  for the singlet and  $\sqrt{2}\sin\sqrt{2}\phi_\sigma, \exp(\mp i\sqrt{2}\theta_\sigma)$  for the triplet state.<sup>15)</sup> Using eqs. (8) and (13), it can be seen that the fermion operator should satisfy the anti-periodic boundary conditions (APBC) for these excitations:  $\psi_{r,\sigma}(x+L) = -\psi_{r,\sigma}(x)$ . This indicates that APBC plays a role in the elimination of the induced charge excitations.<sup>16)</sup>

The effect of the backward scattering term with the coupling  $g_{1\perp}$  is considered using a renormalization group analysis under the change of the cutoff  $a \rightarrow e^{dl}a$ , then the scaling dimensions of the singlet ( $x_{\sigma s}$ ) and the triplet ( $x_{\sigma t}$ ) excitations split logarithmically by the marginally irrelevant coupling  $y_0(l) \equiv g_{1\perp}/\pi v_\sigma$  as<sup>15,17)</sup>

$$x_{\sigma s} = \frac{1}{2} + \frac{3}{4} \frac{y_0}{y_0 \ln L + 1}, \quad (14a)$$

$$x_{\sigma t} = \frac{1}{2} - \frac{1}{4} \frac{y_0}{y_0 \ln L + 1}, \quad (14b)$$

where  $y_0$  is the bare coupling  $y_0 \equiv y_0(l=0)$ . In the TL region where the backward scattering is repulsive ( $y_0 > 0$ ),  $g_{1\perp}$  is renormalized to 0. On the other hand, when the backward scattering becomes attractive ( $y_0 < 0$ ),  $g_{1\perp}$  is renormalized to  $-\infty$  and a spin gap appears. At the critical point  $y_0 = 0$ , there are no logarithmic corrections. Thus, the critical point is determined with high-accuracy by the intersection of these spectra. This way of determination of the spin-gap phase boundary is equivalent to the spin-gap generation in the theory of TL liquids.<sup>10)</sup>

Fig. 1(a) shows the phase diagram of eq.(1) at  $\alpha = 1/2$ . The exponent  $K_\rho$  is calculated in the  $L = 16$  system in a similar manner as shown by Ogata *et al.*, which was used for the  $t$ - $J$ (- $J'$ ) model.<sup>7,18,19)</sup> The phase boundary starts from the critical value of the low-density limit, and bends at  $n \sim 2/3$ . It then flows into the critical point of the  $J, J' \rightarrow 0$  limit. Thus the spin-gap phase appears near half-filling, and in the large  $J/t$  region as in the  $t$ - $J$  model, but it has a single domain in the phase diagram. Ogata *et al.* estimated that the  $J/t$  dependence of the spin-gap phase in the low-doping region is small, and observed the spin gap in the large  $J/t$  region at  $n = 2/3$  using a finite-size scaling method.<sup>7)</sup> These estimations are almost consistent with our results.

Another interesting feature of the phase diagram is that the spin-gap phase boundary overlaps the  $K_\rho = 1$  line where the TL liquid behaves as free electrons in the low density region. This point will be clarified later in connection with the two-electron problem.

In the theory of TL liquids, both the singlet and the triplet superconducting correlations (SS, TS) have the same critical exponent  $1/K_\rho + 1$ ,<sup>10)</sup> but TS is dominant if the logarithmic corrections are taken into account.<sup>15)</sup> However, in the presence of the spin gap, SS is enhanced to  $1/K_\rho$  and TS decays exponentially.<sup>7)</sup> In the case of the  $t$ - $J$  model ( $\alpha = 0$ ), the spin-gap phase boundary lies in the  $K_\rho > 1$  region<sup>1,18)</sup>(see Fig. 1(c)). On the other hand, at  $\alpha = 1/2$  it lies in the  $K_\rho < 1$  region, so that there is no TS region in the latter case.

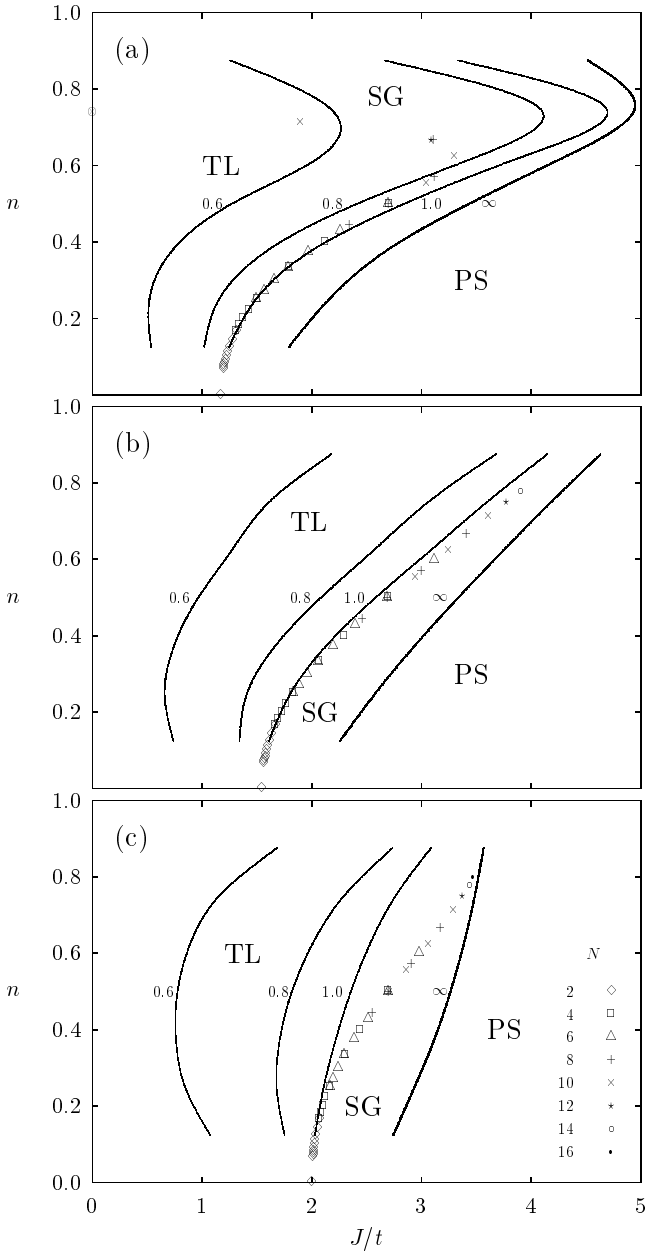


Fig. 1. Phase diagram of the 1D  $t$ - $J$ - $J'$  model at (a)  $\alpha = 1/2$ , (b)  $\alpha = 0.2411$ , (c)  $\alpha = 0$  (TL: TL liquid, SG: spin-gap phase, PS: phase-separated state). The spin-gap phase boundary flows into the critical point obtained by the analysis of Ogata *et al.*<sup>7)</sup> (plotted by  $\otimes$  in (a)). The contour lines of  $K_\rho$  are determined by the data of the  $L = 16$  system, based on the analysis of Ogata *et al.*<sup>18,7)</sup>

The phase diagrams for the intermediate values of  $\alpha$  can be constructed in the same way. As an example, we show the phase diagram at  $\alpha = \alpha_c$  in Fig. 1(b). As  $\alpha$  is increased from 0, the spin-gap phase boundary and the phase-separation boundary<sup>20)</sup> shift towards the small  $J/t$  side in the low-density region. On the other hand, in the high-density region, the two lines shift to the larger  $J/t$  side. However, after  $\alpha$  exceeds the value  $\alpha_c$ , the spin-gap phase boundary bends and flows into the point  $(J/t, n) = (0, n_c)$ . The phase separation boundary also goes to the  $J/t \rightarrow 0$  side following the behavior of the spin-gap phase boundary. This behavior indicates

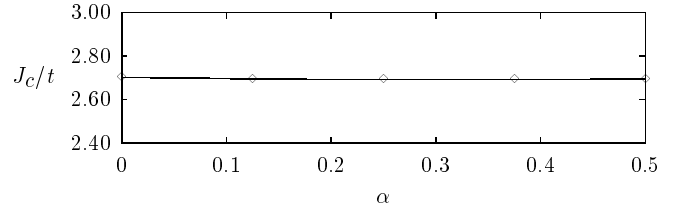


Fig. 2. Critical point  $J_c/t$  versus the strength of the frustration  $\alpha$  in the  $L = 16$  system at  $n = 1/2$ . The critical value is almost constant ( $J_c/t \sim 2.7$ ). This behavior can be explained by applying the  $g$ -ology.

that the phase-separated region is always situated on the border of the spin-gap phase.

In spite of the deformation of the phase diagram, the critical value  $J_c/t$  at the quarter-filling ( $n = 1/2$ ) is almost independent of the strength of the frustration  $\alpha$ , and is kept at  $J_c/t \sim 2.7$  as shown in Fig. 2. Let us consider the reason for this using an argument based on the  $g$ -ology.<sup>10)</sup> In order to apply the  $g$ -ology, we add the on-site Coulomb term  $\mathcal{H}_U$  to eq.(1) and relax the constraint. The original Hamiltonian is restored when we set  $U = \infty$ . The interaction term in eq.(1) is divided into the XY and Ising terms as

$$\mathcal{H}_{XY}^{(l)} = \frac{J^{(l)}}{2} \sum_i (S_i^+ S_{i+l}^- + S_i^- S_{i+l}^+), \quad (15a)$$

$$\mathcal{H}_{\text{Ising}}^{(l)} = -\frac{J^{(l)}}{2} \sum_i (n_{i\uparrow} n_{i+l\downarrow} + n_{i\downarrow} n_{i+l\uparrow}). \quad (15b)$$

Since the  $g$ -ology is appropriate for the weak coupling case, we consider the  $l = 2$  terms of eq.(15) as corrections to the  $t$ - $J$  model which belongs to the universality class of the TL model. Then their contributions to the  $g$ -parameters, which are related to the spin-gap generation, are identified as<sup>10)</sup>

$$\delta g_{1\perp} = \delta g_{1\parallel} = -J'(1 + \cos 4k_F). \quad (16)$$

Note that the  $g$ -parameters are redefined as  $g_{1\parallel} - g_{2\parallel} + g_{2\perp} \rightarrow g_{1\parallel}$ . For the quarter-filling, eq.(16) vanishes, so that the  $l = 2$  terms of eq.(15) do not affect the renormalization flow of the spin part. Thus the frustration does not change the critical point at the quarter-filling within the scheme of the  $g$ -ology.

Finally, we discuss the equivalence between the level-crossing method and the solution of the two-electron problem,<sup>9)</sup> and the accordance between the spin-gap phase boundary and the  $K_\rho = 1$  line in the low-density region. In the low-density limit, the many-body problem can be reduced to a two-body problem. The wave function of the two-electron system is given by

$$\Psi = \sum_{ij} \Phi(i, j) c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger |vac\rangle, \quad (17)$$

where  $\Phi(i, j) = \Phi(j, i)$  for the singlet and  $\Phi(i, j) = -\Phi(j, i)$  for the triplet state. It is well-known that for a two-body problem the ground state is a singlet state as far as the bottom of the energy band has no degeneracy.<sup>21, 22)</sup> For periodic boundary conditions, the singlet

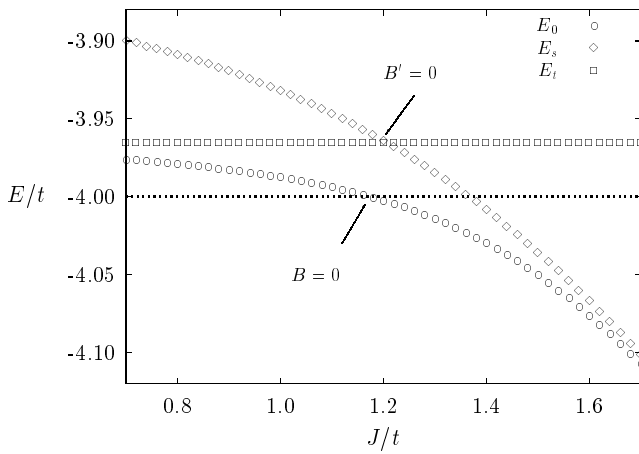


Fig. 3. Ground state energy ( $E_0$ ) and the first singlet and the triplet excitation spectra ( $E_s, E_t$ ) of the two-electron system with length  $L = 24$  at  $\alpha = 1/2$ .  $E_s$  and  $E_t$  are calculated using anti-periodic boundary conditions. The marked intersections will coincide in the  $L \rightarrow \infty$  limit.

ground state energy is given by  $E_0 = -4t + B$  where  $B$  is the bound energy, and the critical value where  $B = 0$  is given by eq.(4) without size dependence. However, for APBC, the bottom of the energy band is degenerate, so that the triplet state can be the ground state. One can show that there is no effect of  $J^{(l)}$  for the triplet state. Then the lowest energy of the triplet state for APBC is always  $E_t = -4t + \delta(L)$  where  $\delta(L) \equiv 8t \sin^2(\pi/2L)$ . On the other hand, the energy for the singlet state for APBC is given by  $E_s = -4t + \delta(L) + B'$  where  $B'$  is the bound energy. Then the level-crossing between the two levels takes place at  $B' = 0$  (see Fig. 3). In the thermodynamic limit,  $\delta(L \rightarrow \infty) = 0$  and the difference between boundary conditions should vanish. This means that the critical points for  $B = 0$  and  $B' = 0$  will be the same in the thermodynamic limit. In this way, it turns out that the singlet-triplet level-cross point is nothing but the solution of the two-electron problem ( $B = 0$ ) in the low-density limit.

In the TL liquid theory electrons behave as free particles at  $K_\rho = 1$ , so that the spin-gap phase boundary, where the bound energy becomes 0, should overlap the  $K_\rho = 1$  line in the low-density limit. Moreover, since the system in the  $J < J_c$  region is equivalent to the non-interacting spinless fermion system ( $K_\rho = 0.5$ ), the contour lines for  $0.5 < K_\rho < 1$  will focus on the point  $(J_c/t, 0)$ .

In conclusion, we studied the spin-gap phase of the 1D  $t$ - $J$ - $J'$  model using the singlet-triplet level-crossing method with the twisted boundary conditions. The obtained results show remarkable consistency with the exactly known results. The spin-gap phase appears near the half-filling as expected, and also appears as a precursor of the phase separation as in the  $t$ - $J$  model. The spin-gap phase has a single domain in the phase diagram. The overlap between the spin-gap phase boundary and the  $K_\rho = 1$  line in the low density region is explained in the connection with the two-electron problem.

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